

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.38	167.59

=> d his

(FILE 'HOME' ENTERED AT 12:43:29 ON 14 JUN 2006)

FILE 'REGISTRY' ENTERED AT 12:44:03 ON 14 JUN 2006

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L1      STRUCTURE UPLOADED
L2      0 S L1
L3      0 S L1 FULL

```

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.38	167.59

FILE 'REGISTRY' ENTERED AT 12:49:35 ON 14 JUN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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STRUCTURE FILE UPDATES: 13 JUN 2006 HIGHEST RN 887650-39-7
 DICTIONARY FILE UPDATES: 13 JUN 2006 HIGHEST RN 887650-39-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

```

*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****

```

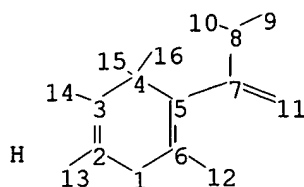
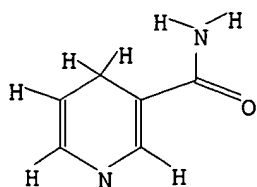
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10099830_2.str



17

```
chain nodes :
7  8  9 10 11 12 13 14 15 16 17
ring nodes :
1  2  3  4  5  6
chain bonds :
2-13 3-14 4-15 4-16 5-7 6-12 7-8 7-11 8-9 8-10
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11
exact bonds :
2-13 3-14 4-15 4-16 5-7 6-12 8-9 8-10
```

Match level :

```
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
```

L4 STRUCTURE UPLOADED

=> s 14 full

FULL SEARCH INITIATED 12:49:51 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 226903 TO ITERATE

100.0% PROCESSED 226903 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.02

L5 0 SEA SSS FUL L4

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

334.53

STN INTERNATIONAL LOGOFF AT 12:50:07 ON 14 JUN 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1642BJF

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1	Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	"Ask CAS" for self-help around the clock
NEWS	3 JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	4 FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	5 FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	6 FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	7 FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	8 MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	9 MAR 22	EMBASE is now updated on a daily basis
NEWS	10 APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	11 APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	12 APR 04	STN AnaVist \$500 visualization usage credit offered
NEWS	13 APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	14 APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	15 APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS	16 MAY 10	CA/CAPLUS enhanced with 1900-1906 U.S. patent records
NEWS	17 MAY 11	KOREAPAT updates resume
NEWS	18 MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS	19 MAY 30	IPC 8 Rolled-up Core codes added to CA/CAPLUS and USPTFULL/USPAT2
NEWS	20 MAY 30	The F-Term thesaurus is now available in CA/CAPLUS
NEWS	21 JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS		FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 14 Jun 2006 VOL 144 ISS 25

FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s us 20030086933/pn

L1 1 US 20030086933/PN
(US2003086933/PN)

=> sel rn

E1 THROUGH E45 ASSIGNED

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.49	2.70

FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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STRUCTURE FILE UPDATES: 13 JUN 2006 HIGHEST RN 887650-39-7

DICTIONARY FILE UPDATES: 13 JUN 2006 HIGHEST RN 887650-39-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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```

*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****

```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> s e1-e45

```

1 19132-12-8/BI
  (19132-12-8/RN)
1 21919-05-1/BI
  (21919-05-1/RN)
1 100-39-0/BI
  (100-39-0/RN)
1 106-94-5/BI
  (106-94-5/RN)
1 106047-77-2/BI
  (106047-77-2/RN)
1 107-08-4/BI
  (107-08-4/RN)
1 109942-74-7/BI
  (109942-74-7/RN)
1 1120-71-4/BI
  (1120-71-4/RN)
1 114554-11-9/BI
  (114554-11-9/RN)
1 115503-79-2/BI
  (115503-79-2/RN)
1 119643-82-2/BI
  (119643-82-2/RN)
1 126298-92-8/BI
  (126298-92-8/RN)
1 141-76-4/BI
  (141-76-4/RN)
1 144-48-9/BI
  (144-48-9/RN)
1 17376-04-4/BI
  (17376-04-4/RN)
1 17750-23-1/BI
  (17750-23-1/RN)
1 17750-24-2/BI
  (17750-24-2/RN)
1 218443-88-0/BI
  (218443-88-0/RN)
1 218443-90-4/BI
  (218443-90-4/RN)
1 218443-91-5/BI
  (218443-91-5/RN)
1 218443-92-6/BI
  (218443-92-6/RN)
1 218443-93-7/BI
  (218443-93-7/RN)

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1 4229-56-5/BI
 (4229-56-5/RN)
 1 51652-08-5/BI
 (51652-08-5/RN)
 1 52047-79-7/BI
 (52047-79-7/RN)
 1 53-57-6/BI
 (53-57-6/RN)
 1 5463-59-2/BI
 (5463-59-2/RN)
 1 58-68-4/BI
 (58-68-4/RN)
 1 58880-44-7/BI
 (58880-44-7/RN)
 1 624-76-0/BI
 (624-76-0/RN)
 1 627-18-9/BI
 (627-18-9/RN)
 1 6456-44-6/BI
 (6456-44-6/RN)
 1 64881-21-6/BI
 (64881-21-6/RN)
 1 667919-86-0/BI
 (667919-86-0/RN)
 1 7145-37-1/BI
 (7145-37-1/RN)
 1 72306-81-1/BI
 (72306-81-1/RN)
 1 75-03-6/BI
 (75-03-6/RN)
 1 75-26-3/BI
 (75-26-3/RN)
 1 75-30-9/BI
 (75-30-9/RN)
 1 89080-16-0/BI
 (89080-16-0/RN)
 1 9037-41-6/BI
 (9037-41-6/RN)
 1 952-92-1/BI
 (952-92-1/RN)
 1 97009-81-9/BI
 (97009-81-9/RN)
 1 98-92-0/BI
 (98-92-0/RN)
 1 99362-74-0/BI
 (99362-74-0/RN)

L2 45 (19132-12-8/BI OR 21919-05-1/BI OR 100-39-0/BI OR 106-94-5/BI
 OR 106047-77-2/BI OR 107-08-4/BI OR 109942-74-7/BI OR 1120-71-4/
 BI OR 114554-11-9/BI OR 115503-79-2/BI OR 119643-82-2/BI OR 12629
 8-92-8/BI OR 141-76-4/BI OR 144-48-9/BI OR 17376-04-4/BI OR 17750
 -23-1/BI OR 17750-24-2/BI OR 218443-88-0/BI OR 218443-90-4/BI OR
 218443-91-5/BI OR 218443-92-6/BI OR 218443-93-7/BI OR 4229-56-5/B
 I OR 51652-08-5/BI OR 52047-79-7/BI OR 53-57-6/BI OR 5463-59-2/BI
 OR 58-68-4/BI OR 58880-44-7/BI OR 624-76-0/BI OR 627-18-9/BI OR
 6456-44-6/BI OR 64881-21-6/BI OR 667919-86-0/BI OR 7145-37-1/BI
 OR 72306-81-1/BI OR 75-03-6/BI OR 75-26-3/BI OR 75-30-9/BI OR
 89080-16-0/BI OR 9037-41-6/BI OR 952-92-1/BI OR 97009-81-9/BI OR
 98-92-0/BI OR 99362-74-0/BI)

=> d 1-45

L2 ANSWER 1 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 667919-86-0 REGISTRY
 ED Entered STN: 26 Mar 2004

CN Dehydrogenase, reduced nicotinamide riboside (quinone) (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Dihydronicotinamide riboside quinone oxidoreductase 2
CN Dihydronicotinamide riboside quinone reductase 2
CN Dihydronicotinamide riboside:quinone oxidoreductase
CN NQO2 oxidoreductase
CN NRH:quinone oxidoreductase
CN Quinone reductase 2
CN Reduced nicotinamide riboside (quinone) dehydrogenase
MF Unspecified
CI MAN
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

39 REFERENCES IN FILE CA (1907 TO DATE)

39 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN

RN **218443-93-7** REGISTRY

ED Entered STN: 29 Jan 1999

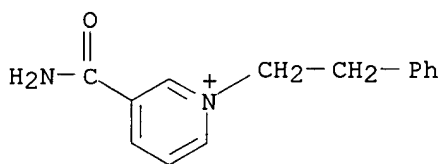
CN Pyridinium, 3-(aminocarbonyl)-1-(2-phenylethyl)-, iodide (9CI) (CA INDEX NAME)

MF C14 H15 N2 O . I

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CRN (761385-40-4)



● I⁻

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 3 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN

RN **218443-92-6** REGISTRY

ED Entered STN: 29 Jan 1999

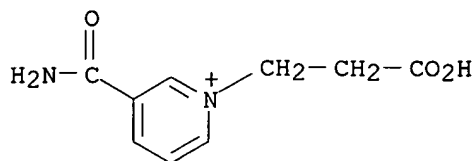
CN Pyridinium, 3-(aminocarbonyl)-1-(2-carboxyethyl)-, iodide (9CI) (CA INDEX NAME)

MF C9 H11 N2 O3 . I

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

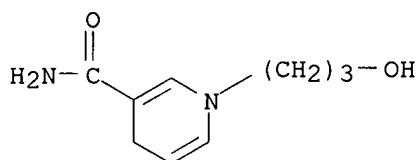
CRN (717820-87-6)



● I⁻

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

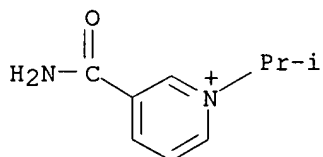
L2 ANSWER 4 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-91-5** REGISTRY
ED Entered STN: 29 Jan 1999
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(3-hydroxypropyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H14 N2 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

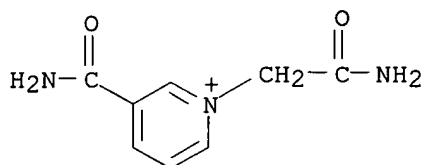
L2 ANSWER 5 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-90-4** REGISTRY
ED Entered STN: 29 Jan 1999
CN Pyridinium, 3-(aminocarbonyl)-1-(1-methylethyl)-, bromide (9CI) (CA INDEX NAME)
MF C9 H13 N2 O . Br
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (745779-44-6)



● Br⁻

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

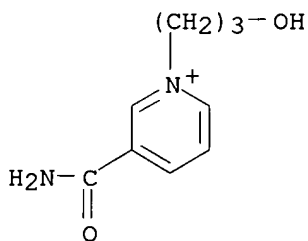
L2 ANSWER 6 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **218443-88-0** REGISTRY
ED Entered STN: 29 Jan 1999
CN Pyridinium, 3-(aminocarbonyl)-1-(2-amino-2-oxoethyl)-, iodide (9CI) (CA INDEX NAME)
MF C8 H10 N3 O2 . I
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (66822-26-2)



● I⁻

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 7 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **126298-92-8** REGISTRY
ED Entered STN: 06 Apr 1990
CN Pyridinium, 3-(aminocarbonyl)-1-(3-hydroxypropyl)-, bromide (9CI) (CA INDEX NAME)
MF C9 H13 N2 O2 . Br
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
CRN (83643-85-0)

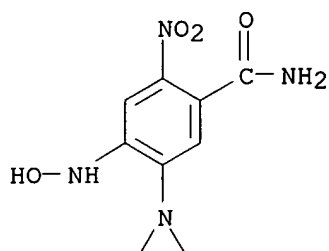


● Br⁻

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 8 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **119643-82-2** REGISTRY
ED Entered STN: 17 Mar 1989
CN Benzamide, 5-(1-aziridinyl)-4-(hydroxyamino)-2-nitro- (9CI) (CA INDEX NAME)

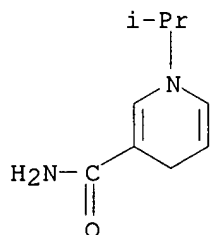
FS 3D CONCORD
 MF C9 H10 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)
 13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

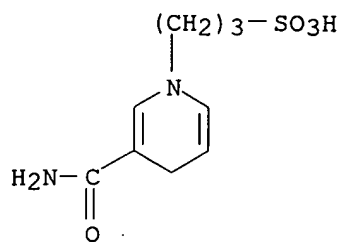
L2 ANSWER 9 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **115503-79-2** REGISTRY
 ED Entered STN: 30 Jul 1988
 CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(1-methylethyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C9 H14 N2 O
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

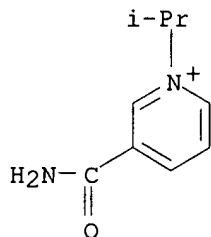
L2 ANSWER 10 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **114554-11-9** REGISTRY
 ED Entered STN: 21 May 1988
 CN 1(4H)-Pyridinepropanesulfonic acid, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 1(4H)-Pyridinepropanesulfonic acid, 3-carbamoyl- (6CI)
 FS 3D CONCORD
 MF C9 H14 N2 O4 S
 SR CAOLD
 LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

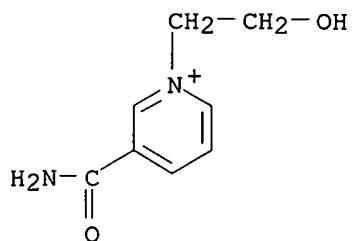
L2 ANSWER 11 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **109942-74-7** REGISTRY
 ED Entered STN: 22 Aug 1987
 CN Pyridinium, 3-(aminocarbonyl)-1-(1-methylethyl)-, iodide (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Carbamoyl-1-isopropylpyridinium iodide (6CI)
 MF C9 H13 N2 O . I
 SR CAOLD
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 CRN (745779-44-6)



● I⁻

5 REFERENCES IN FILE CA (1907 TO DATE)
 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

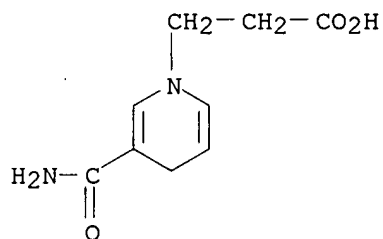
L2 ANSWER 12 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **106047-77-2** REGISTRY
 ED Entered STN: 10 Jan 1987
 CN Pyridinium, 3-(aminocarbonyl)-1-(2-hydroxyethyl)-, iodide (9CI) (CA INDEX NAME)
 MF C8 H11 N2 O2 . I
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
 CRN (66822-21-7)



● I⁻

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

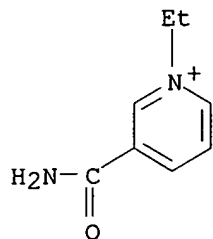
L2 ANSWER 13 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **99362-74-0** REGISTRY
ED Entered STN: 07 Dec 1985
CN 1(4H)-Pyridinepropanoic acid, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1(4H)-Pyridinepropionic acid, 3-carbamoyl- (6CI)
FS 3D CONCORD
MF C9 H12 N2 O3
SR CAOLD
LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

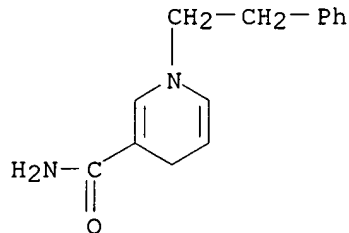
L2 ANSWER 14 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **97009-81-9** REGISTRY
ED Entered STN: 01 Jul 1985
CN Pyridinium, 3-(aminocarbonyl)-1-ethyl-, iodide (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-ethylpyridinium iodide (6CI)
CN Pyridinium, 3-carbamyl-1-ethyl-, iodide (4CI)
MF C8 H11 N2 O . I
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
CRN (71413-64-4)



● I⁻

12 REFERENCES IN FILE CA (1907 TO DATE)
 12 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

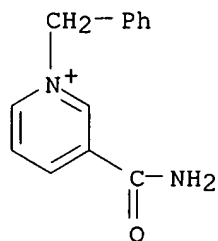
L2 ANSWER 15 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **89080-16-0** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C14 H16 N2 O
 LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 16 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **72306-81-1** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Pyridinium, 3-(aminocarbonyl)-1-(phenylmethyl)-, iodide (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 1-Benzyl-3-carbamoylpyridinium iodide (6CI, 7CI)
 MF C13 H13 N2 O . I
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 CRN (16183-83-8)

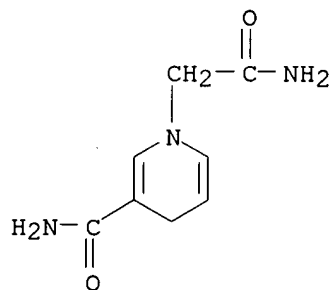


● I⁻

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 17 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **64881-21-6** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 1(4H)-Pyridineacetamide, 3-(aminocarbonyl)- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 1-Carbamoylmethyl-1,4-dihydronicotinamide
 CN Caricotamide
 CN EP 0152R
 FS 3D CONCORD
 MF C8 H11 N3 O2
 LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USAN, USPATFULL
 (*File contains numerically searchable property data)

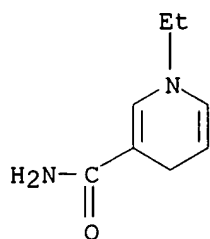


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
 9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 18 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **58880-44-7** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 3-Pyridinecarboxamide, 1-ethyl-1,4-dihydro- (9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN N-Ethyl-1,4-dihydronicotinamide
 FS 3D CONCORD
 MF C8 H12 N2 O
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 19 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN

RN **52047-79-7** REGISTRY

ED Entered STN: 16 Nov 1984

CN Pyridinium, 3-(aminocarbonyl)-1-propyl-, bromide (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyridinium, 3-carbamoyl-1-propyl-, bromide (6CI)

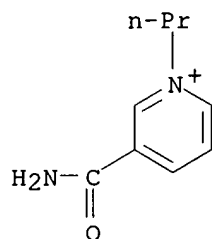
OTHER NAMES:

CN 3-Carbamoyl-1-propylpyridinium bromide

MF C9 H13 N2 O . Br

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

CRN (13309-33-6)



● Br⁻

15 REFERENCES IN FILE CA (1907 TO DATE)

15 REFERENCES IN FILE CAPLUS (1907 TO DATE)

4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 20 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN

RN **51652-08-5** REGISTRY

ED Entered STN: 16 Nov 1984

CN Pyridinium, 3-(aminocarbonyl)-1-(3-sulfopropyl)-, inner salt (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3-Carbamoyl-1-(3-sulfopropyl)pyridinium hydroxide, inner salt (6CI)

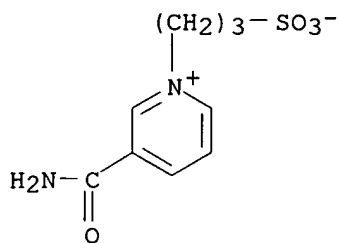
CN Pyridinium, 3-(aminocarbonyl)-1-(3-sulfopropyl)-, hydroxide, inner salt

FS 3D CONCORD

MF C9 H12 N2 O4 S

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMLIST, MSDS-OHS,
TOXCENTER, USPATFULL

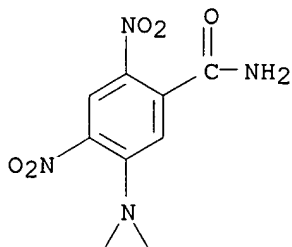
(*File contains numerically searchable property data)
 Other Sources: EINECS**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)
 11 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 21 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 21919-05-1 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Benzamide, 5-(1-aziridinyl)-2,4-dinitro- (8CI, 9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 2,4-Dinitro-5-ethyleneiminobenzamide
 CN 2,4-Dinitroethyleneiminobenzamide
 CN 5-(1-Aziridinyl)-2,4-dinitrobenzamide
 CN 5-Aziridino-2,4-dinitrobenzamide
 CN 5-Aziridinyl-2,4-dinitrobenzamide
 CN CB 1954
 CN NSC 115829
 CN Tretazicar
 MF C9 H8 N4 O5
 LC STN Files: ADISNEWS, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CHEMCATS, CIN, CSCHM, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSRESEARCH, MEDLINE, PROMT, PROUSDDR, RTECS*, TOXCENTER, USAN, USPAT2, USPATFULL
 (*File contains numerically searchable property data)



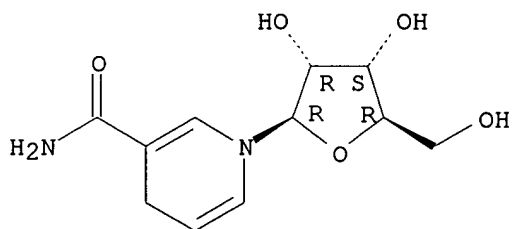
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

176 REFERENCES IN FILE CA (1907 TO DATE)
 5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 176 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 22 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 19132-12-8 REGISTRY

ED Entered STN: 16 Nov 1984
 CN 3-Pyridinecarboxamide, 1,4-dihydro-1-β-D-ribofuranosyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Nicotinamide, 1,4-dihydro-1-β-D-ribofuranosyl- (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN β-Reduced nicotinamide ribonucleoside
 CN Reduced nicotinamide riboside
 FS STEREOSEARCH
 MF C11 H16 N2 O5
 CI COM
 LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)

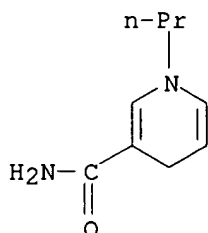
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

16 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 16 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

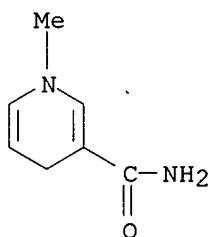
L2 ANSWER 23 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 17750-24-2 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 3-Pyridinecarboxamide, 1,4-dihydro-1-propyl- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Nicotinamide, 1,4-dihydro-1-propyl- (6CI, 7CI, 8CI)
 OTHER NAMES:
 CN 1,4-Dihydro-N1-propylnicotinamide
 CN 1-n-Propyl-1,4-dihydronicotinamide
 CN 1-Propyl-1,4-dihydronicotinamide
 CN N-Propyldihydronicotinamide
 CN N1-(n-Propyl)-1,4-dihydronicotinamide
 FS 3D CONCORD
 MF C9 H14 N2 O
 LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

96 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
96 REFERENCES IN FILE CAPLUS (1907 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 24 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **17750-23-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-methyl- (6CI, 8CI)
OTHER NAMES:
CN 1,4-Dihydro-1-methylnicotinamide
CN 1,4-Dihydro-N-methylnicotinamide
CN 1-Methyl-1,4-dihydronicotinamide
CN 3-Carbamoyl-1,4-dihydro-1-methylpyridine
CN N-Methyl-1,4-dihydronicotinamide
FS 3D CONCORD
MF C7 H10 N2 O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
IFICDB, IFIPAT, IFIUDB, MEDLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

107 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
107 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 25 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **17376-04-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzene, (2-iodoethyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN (2-Iodoethyl)benzene
CN β -Phenethyl iodide
CN β -Phenylethyl iodide
CN 1-Iodo-2-phenylethane
CN 2-Phenylethyl iodide
CN Phenethyl iodide
FS 3D CONCORD
MF C8 H9 I
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, SPECINFO, TOXCENTER,
USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

ICH₂-CH₂-Ph

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

281 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
282 REFERENCES IN FILE CAPLUS (1907 TO DATE)
15 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

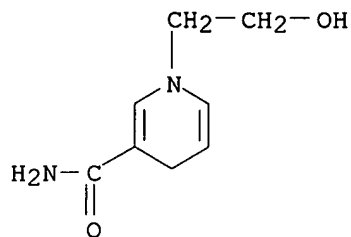
L2 ANSWER 26 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **9037-41-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN Reductase, nitro- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2,4,6-Trinitrotoluene nitroreductase
CN 3-Nitrophenol reductase
CN 4-Nitrobiphenyl reductase
CN Aromatic nitroreductase
CN Dinitropyrene nitroreductase
CN Nitrobenzene nitroreductase
CN Nitrobenzene reductase
CN Nitrobenzoic acid reductase
CN Nitrophenol reductase
CN Nitroreductase
CN Nitroreductase (NADH)
CN PETN reductase
CN TNT nitroreductase
MF Unspecified
CI MAN
LC STN Files: ADISNEWS, AGRICOLA, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT,
CIN, EMBASE, PIRA, PROMT, TOXCENTER, USPAT2, USPATFULL

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

679 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
680 REFERENCES IN FILE CAPLUS (1907 TO DATE)

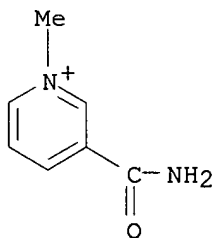
L2 ANSWER 27 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **7145-37-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(2-hydroxyethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Nicotinamide, 1,4-dihydro-1-(2-hydroxyethyl)- (7CI, 8CI)
OTHER NAMES:
CN NSC 74259
FS 3D CONCORD
MF C8 H12 N2 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 28 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **6456-44-6** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Pyridinium, 3-(aminocarbonyl)-1-methyl-, iodide (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Carbamoyl-1-methylpyridinium iodide (6CI, 7CI)
 CN Pyridinium, 3-carbamoyl-1-methyl-, iodide (8CI)
 CN Pyridinium, 3-carbamyl-1-methyl-, iodide (4CI)
 OTHER NAMES:
 CN 1-Methylnicotinamide iodide
 CN Nicotinamide methiodide
 MF C7 H9 N2 O . I
 CI COM
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST,
 CSCHEM, GMELIN*, RTECS*, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**
 (**Enter CHEMLIST File for up-to-date regulatory information)
 CRN (3106-60-3)

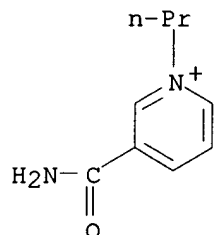


● I⁻

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

104 REFERENCES IN FILE CA (1907 TO DATE)
 104 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 19 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 29 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **5463-59-2** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Pyridinium, 3-(aminocarbonyl)-1-propyl-, iodide (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 3-Carbamoyl-1-propylpyridinium iodide (6CI, 7CI)
 CN Pyridinium, 3-carbamoyl-1-propyl-, iodide (8CI)
 MF C9 H13 N2 O . I
 LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)
 CRN (13309-33-6)

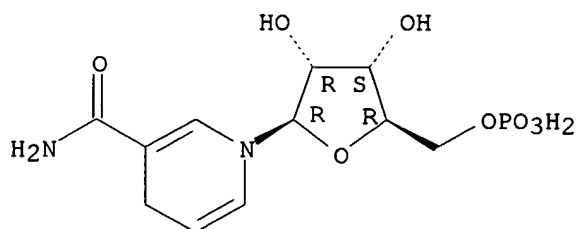


● I⁻

18 REFERENCES IN FILE CA (1907 TO DATE)
 18 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 30 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN **4229-56-5** REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(5-O-phosphono-β-D-ribofuranosyl)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Nicotinamide, 1,4-dihydro-1-β-D-ribofuranosyl-, 5'-(dihydrogen phosphate) (8CI)
 CN Nicotinamide, 1,4-dihydro-1-β-D-ribofuranosyl-, 5'-phosphate (7CI)
 OTHER NAMES:
 CN β-NMNH
 CN 1,4-Dihydronicotinamide mononucleotide
 CN 1,4-Dihydronicotinamide ribonucleotide
 CN Nicotinamide ribonucleotide, reduced
 CN NMNH
 CN NMNH2
 CN Reduced nicotinamide mononucleotide
 CN Reduced nicotinamide ribonucleotide
 FS STEREOSEARCH
 MF C11 H17 N2 O8 P
 CI COM
 LC STN Files: AGRICOLA, BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER, USPATFULL
 (*File contains numerically searchable property data)

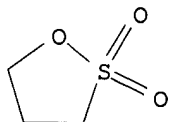
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

77 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 77 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 31 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 1120-71-4 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 1,2-Oxathiolane, 2,2-dioxide (8CI, 9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 1-Propanesulfonic acid, 3-hydroxy-, γ -sultone (6CI)
 OTHER NAMES:
 CN γ -Propane sultone
 CN 1,3-Propane sultone
 CN 1,3-Trimethylene sultone
 CN 3-Hydroxy-1-propanesulfonic acid γ -sultone
 CN 3-Hydroxy-1-propanesulfonic acid sultone
 CN NSC 42386
 CN Propane sultone
 CN Propyl sultone
 FS 3D CONCORD
 MF C3 H6 O3 S
 CI COM
 LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHM, CSNB, DETHERM*, EMBASE, ENCOMPAT, ENCOMPAT2, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1761 REFERENCES IN FILE CA (1907 TO DATE)
 383 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1765 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 31 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 32 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **952-92-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 3-Pyridinecarboxamide, 1,4-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Nicotinamide, 1-benzyl-1,4-dihydro- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 1,4-Dihydro-1-(phenylmethyl)-3-pyridinecarboxamide

CN 1,4-Dihydro-N-benzylnicotinamide

CN 1-Benzyl-1,4-dihydronicotinamide

CN 1-Benzyl-3-carbamido-1,4-dihydropyridine

CN 1-Benzyl-3-carbamoyl-1,4-dihydropyridine

CN BNAH

CN N-Benzyl-1,4-dihydronicotinamide

CN N-Benzyl-3-carbamoyl-1,4-dihydropyridine

CN N-Benzylidihydronicotinamide

CN NSC 26899

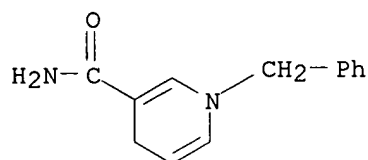
FS 3D CONCORD

DR 174307-50-7, 84062-23-7

MF C13 H14 N2 O

CI COM

LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, MEDLINE, PIRA, PROMT, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

584 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

584 REFERENCES IN FILE CAPLUS (1907 TO DATE)

31 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 33 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **627-18-9** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Propanol, 3-bromo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1-Bromo-3-hydroxypropane

CN 1-Bromo-3-propanol

CN 3-Bromo-1-propanol

CN 3-Bromopropyl alcohol

CN 3-Hydroxypropyl bromide

CN Trimethylene bromohydrin

FS 3D CONCORD

MF C3 H7 Br O

CI COM

LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)

Other Sources: EINECS**, NDSL**, TSCA**
(*Enter CHEMLIST File for up-to-date regulatory information)

Br-CH₂-CH₂-CH₂-OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1404 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1409 REFERENCES IN FILE CAPLUS (1907 TO DATE)
8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 34 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **624-76-0** REGISTRY
ED Entered STN: 16 Nov 1984
CN Ethanol, 2-iodo- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Iodoethanol
CN Ethylene iodohydrin
CN Iodoethanol
CN NSC 85227
FS 3D CONCORD
MF C2 H5 I O
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, IFICDB, IFIPAT, IFIUDB,
RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(*Enter CHEMLIST File for up-to-date regulatory information)

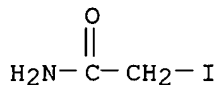
I-CH₂-CH₂-OH

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

477 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
477 REFERENCES IN FILE CAPLUS (1907 TO DATE)
7 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 35 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **144-48-9** REGISTRY
ED Entered STN: 16 Nov 1984
CN Acetamide, 2-iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetamide, iodo- (6CI)
OTHER NAMES:
CN α-Iodoacetamide
CN 2-Iodoacetamide
CN Iodoacetamide
CN Monoiodoacetamide
CN NSC 9581
CN Surauto
FS 3D CONCORD
MF C2 H4 I N O
CI COM
LC STN Files: AGRICOLA, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD,
CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DDFU, DRUGU,

EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MSDS-OHS, NAPRALERT, PIRA,
PROMT, RTECS*, SCISEARCH, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1651 REFERENCES IN FILE CA (1907 TO DATE)
46 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1654 REFERENCES IN FILE CAPLUS (1907 TO DATE)
80 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 36 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **141-76-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propanoic acid, 3-iodo- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Propionic acid, 3-iodo- (6CI, 7CI, 8CI)
OTHER NAMES:
CN β -Iodopropionic acid
CN 3-Iodopropanoic acid
CN 3-Iodopropionic acid
CN NSC 2124
FS 3D CONCORD
MF C3 H5 I O2
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, MSDS-OHS, RTECS*,
SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

183 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
183 REFERENCES IN FILE CAPLUS (1907 TO DATE)
17 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 37 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **107-08-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 1-iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Iodopropane
CN n-Propyl iodide
CN Propane iodide
CN Propyl iodide
FS 3D CONCORD
MF C3 H7 I

CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, DETHERM*, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIADB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

CCCI

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3224 REFERENCES IN FILE CA (1907 TO DATE)
13 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3230 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 38 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN 106-94-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 1-bromo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Bromopropane
CN 1-Propyl bromide
CN Ascusol MC
CN Leksol
CN n-Propyl bromide
CN Propyl bromide
FS 3D CONCORD
MF C3 H7 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIADB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

BrCCC

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4243 REFERENCES IN FILE CA (1907 TO DATE)
46 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
4250 REFERENCES IN FILE CAPLUS (1907 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 39 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100-39-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzene, (bromomethyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Toluene, α -bromo- (8CI)

OTHER NAMES:

CN (Bromomethyl)benzene
CN (Bromophenyl)methane
CN α -Bromotoluene
CN ω -Bromotoluene
CN Benzyl bromide
CN NSC 8041
CN Phenylmethyl bromide
FS 3D CONCORD
MF C7 H7 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, PIRA, PROMT, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Ph-CH₂-Br

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13933 REFERENCES IN FILE CA (1907 TO DATE)
106 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
13983 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 40 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN

RN **98-92-0** REGISTRY

ED Entered STN: 16 Nov 1984

CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)

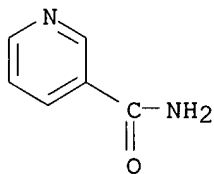
OTHER CA INDEX NAMES:

CN Nicotinamide (8CI)

OTHER NAMES:

CN β -Pyridinecarboxamide
CN 3-(Aminocarbonyl)pyridine
CN 3-Amidopyridine
CN 3-Carbamoylpyridine
CN 3-Pyridinecarboxylic acid amide
CN Aminicotin
CN Benicot
CN Delonin Amide
CN Dipearyl
CN m-(Aminocarbonyl)pyridine
CN NAM
CN Niacinamide
CN Niavit PP
CN Nicamina
CN Nicamindon
CN Nicasir
CN Nicobion
CN Nicofort
CN Nicosan 2
CN Nicosylamide
CN Nicotilamide
CN Nicotine acid amide
CN Nicotinic acid amide
CN Nicotinic amide
CN Nicotylamide

CN Nicovit
 CN Nicovitina
 CN Nictoamide
 CN Niocinamide
 CN Niozymin
 CN NSC 13128
 CN NSC 27452
 CN Papulex
 CN Pelmin
 CN Pelmine
 CN Pelonin amide
 CN Vi-Nicotyl
 CN Vitamin B
 CN Vitamin B3
 FS 3D CONCORD
 DR 123574-63-0, 37321-14-5, 78731-47-2
 MF C6 H6 N2 O
 CI COM
 LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*,
 BIOSIS, BIOTECHNO, CA, CABA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS,
 CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU,
 EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*,
 MSDS-OHS, NAPRALERT, PHAR, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER,
 USAN, USPAT2, USPATFULL, VTB
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**, WHO
 (**Enter CHEMLIST File for up-to-date regulatory information)

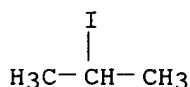


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9281 REFERENCES IN FILE CA (1907 TO DATE)
 409 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 9303 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 41 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
 RN 75-30-9 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN Propane, 2-iodo- (8CI, 9CI) (CA INDEX NAME)
 OTHER NAMES:
 CN 1-Methylethyl iodide
 CN 2-Iodopropane
 CN 2-Propyl iodide
 CN Isopropyl iodide
 CN sec-Propyl iodide
 FS 3D CONCORD
 MF C3 H7 I
 CI COM
 LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT,
 CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, DETHERM*, GMELIN*,
 IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, PS, RTECS*, SPECINFO,
 SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: DSL**, EINECS**, TSCA**

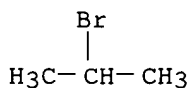
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2962 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2967 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 42 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN 75-26-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Propane, 2-bromo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Bromopropane
CN Isopropyl bromide
CN sec-Propyl bromide
FS 3D CONCORD
MF C3 H7 Br
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, PROMT, PS, RTECS*, SCISEARCH, SPECINFO, SYNTHLINE, TOXCENTER, ULIDAT, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3397 REFERENCES IN FILE CA (1907 TO DATE)
16 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3407 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 43 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN 75-03-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Ethane, iodo- (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl iodide
CN Hydriodic ether
CN Iodoethane
CN Monoiodoethane
CN NSC 8825
FS 3D CONCORD
MF C2 H5 I
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO, CA, CAOLD,

CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, IFICDB, IFIPAT, IFIADB, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

H₃C-CH₂-I

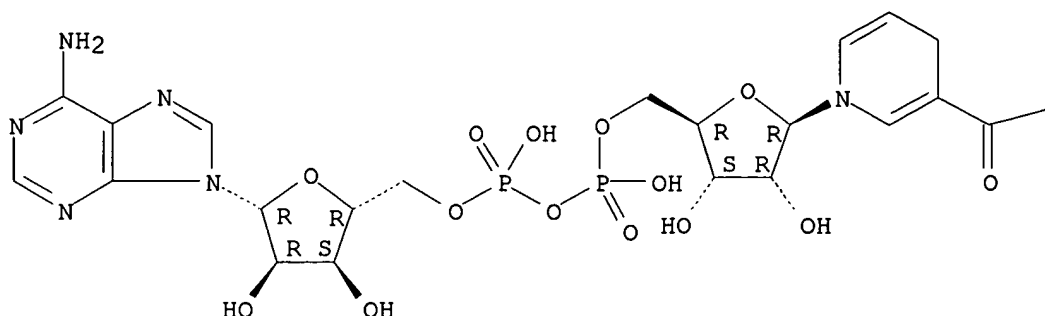
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6901 REFERENCES IN FILE CA (1907 TO DATE)
74 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
6923 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 44 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN
RN **58-68-4** REGISTRY
ED Entered STN: 16 Nov 1984
CN Adenosine 5'-(trihydrogen diphosphate), P'→5'-ester with
1,4-dihydro-1-β-D-ribofuranosyl-3-pyridinecarboxamide (9CI) (CA
INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenosine 5'-(trihydrogen pyrophosphate), 5'→5'-ester with
1,4-dihydro-1-β-D-ribofuranosylnicotinamide (8CI)
CN Adenosine pyrophosphate, 5'→5'-ester with 1,4-dihydro-1-β-D-
ribofuranosylnicotinamide (7CI)
OTHER NAMES:
CN β-DPNH
CN β-NADH
CN 1,4-Dihydronicotinamide adenine dinucleotide
CN Codehydrase I, reduced
CN Codehydrogenase I, reduced
CN Coenzyme I, reduced
CN Cozymase I, reduced
CN Dihydrocodehydrogenase I
CN Dihydrocozymase
CN Dihydronicotinamide adenine dinucleotide
CN Dihydronicotinamide mononucleotide
CN DPNH
CN ENADA
CN NADH
CN NADH2
CN Nicotinamide-adenine dinucleotide, reduced
CN Reduced codehydrogenase I
CN Reduced diphosphopyridine nucleotide
CN Reduced nicotinamide adenine diphosphate
CN Reduced nicotinamide-adenine dinucleotide
FS STEREOSEARCH
DR 443892-10-2
MF C21 H29 N7 O14 P2
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO,
CA, CABA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM,
DDFU, DRUGU, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIADB, MRCK*, PIRA,
PROMT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

—NH₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13781 REFERENCES IN FILE CA (1907 TO DATE)
269 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
13816 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 45 OF 45 REGISTRY COPYRIGHT 2006 ACS on STN

RN **53-57-6** REGISTRY

ED Entered STN: 16 Nov 1984

CN Adenosine 5'-(trihydrogen diphosphate), 2'-(dihydrogen phosphate),
P'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosyl-3-
pyridinecarboxamide (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Adenosine, 2'-(dihydrogen phosphate) 5'-(trihydrogen pyrophosphate),
5'→5'-ester with 1,4-dihydro-1-β-D-ribofuranosylnicotinamide
(8CI)

OTHER NAMES:

CN β-NADPH

CN β-Nicotinamide-adenine-dinucleotide-phosphoric acid

CN β-TPNH

CN 51: PN: WO2004076659 FIGURE: 7 claimed sequence

CN Codehydrase II, reduced

CN Codehydrogenase II, reduced

CN Coenzyme II, reduced

CN Cozymase II, reduced

CN Dihydrocodehydrogenase II

CN NADPH

CN NADPH2

CN Nicotinamide-adenine dinucleotide phosphate, reduced

CN Reduced codehydrogenase II

CN Reduced nicotinamide adenine dinucleotide phosphate

CN Reduced triphosphopyridine nucleotide

CN TPNH

CN Triphosphopyridine nucleotide, reduced

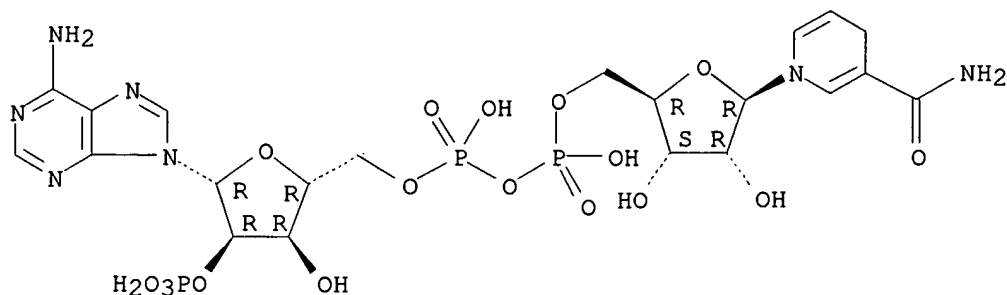
FS STEREOSEARCH

DR 22046-90-8, 3545-01-5

MF C21 H30 N7 O17 P3

CI COM
 LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO,
 CA, CABA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CIN, CSCHEM,
 DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IPA, MRCK*, PROMT,
 TOXCENTER, USPAT2, USPATFULL
 (*File contains numerically searchable property data)
 Other Sources: EINECS**, NDSL**, TSCA**
 (**Enter CHEMLIST File for up-to-date regulatory information)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11386 REFERENCES IN FILE CA (1907 TO DATE)
 239 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 11421 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 57 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
86.82	89.52

FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
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 FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

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=> d his

(FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
L1 1 S US 20030086933/PN
SEL RN

FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
L2 45 S E1-E45

FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006

=> s l2
L3 64271 L2

=> s prodrug (L) l3
10858 PRODRUG
10801 PRODRUGS
15241 PRODRUG
(PRODRUG OR PRODRUGS)
L4 145 PRODRUG (L) L3

=>

=>
Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.87	92.39

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:33:52 ON 14 JUN 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1642BJF

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 14:39:43 ON 14 JUN 2006
FILE 'CAPLUS' ENTERED AT 14:39:43 ON 14 JUN 2006
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.87	92.39

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.33	92.85

FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006
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FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

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=> s 218443-93-7 or 218443-92-6 or 218443-91-5 or 218443-90-4 or 218443-88-0 or 126298-92-8 or 119643-82-2 or 115503-79-2 or 114554-11-9 or 109942-74-7 or 106047-77-2 or 99362-74-0 or 97009-81-9 or 89080-16-0 or 72306-81-1 or 64881-21-6 or 58880-44-7 or 52047-79-7 or 51652-08-5 or 212919-05-1

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L6 4 L5

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L8 12 L7

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L10 3 L9

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L12 4 L11

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L14 5 L13

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L16 3 L15

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L18 5 L17

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L20 13 L19

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L22 4 L21

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L24 3 L23

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L26 2 L25

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L28 2 L27

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L30 2 L29

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L32 2 L31

 2 72306
149422 81
 0 72306-81
 (72306(W)81)

L33 33 L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 OR
 L14 OR L12 OR L10 OR L8 OR L6 OR 72306-81

=> s 17750-23-1 or 7145-37-1 or 6456-44-6 or 5463-59-2 or 4229-56-5 or 952-92-1 or
667919-86-0 or 218443-92-6 or 218443-91-5 or 218443-90-4 or 218443-88-0

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L35 3 L34

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L37 2 L36

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
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L39 2 L38

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
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L41 2 L40

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
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L43 39 L42

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L45 584 L44

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L47 77 L46

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L49 18 L48

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L51 104 L50

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L53 6 L52

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L55 107 L54

L56 878 L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 OR
 L37 OR L35

=> file his
'HIS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CAPLUS'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available. If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

=> d his

(FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
L1 1 S US 20030086933/PN
SEL RN

FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
L2 45 S E1-E45

FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
L3 64271 S L2
L4 145 S PRODRUG (L) L3

FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006
S 218443-93-7/REG# OR 218443-92-6/REG# OR 218443-91-5/REG# OR

FILE 'REGISTRY' ENTERED AT 14:43:18 ON 14 JUN 2006
L5 1 S 89080-16-0/RN

FILE 'CAPLUS' ENTERED AT 14:43:18 ON 14 JUN 2006
L6 4 S L5

FILE 'REGISTRY' ENTERED AT 14:43:19 ON 14 JUN 2006
L7 1 S 97009-81-9/RN

FILE 'CAPLUS' ENTERED AT 14:43:19 ON 14 JUN 2006
L8 12 S L7

FILE 'REGISTRY' ENTERED AT 14:43:20 ON 14 JUN 2006
L9 1 S 99362-74-0/RN

FILE 'CAPLUS' ENTERED AT 14:43:20 ON 14 JUN 2006
L10 3 S L9

FILE 'REGISTRY' ENTERED AT 14:43:21 ON 14 JUN 2006
L11 1 S 106047-77-2/RN

FILE 'CAPLUS' ENTERED AT 14:43:21 ON 14 JUN 2006
L12 4 S L11

FILE 'REGISTRY' ENTERED AT 14:43:22 ON 14 JUN 2006
L13 1 S 109942-74-7/RN

FILE 'CAPLUS' ENTERED AT 14:43:22 ON 14 JUN 2006
L14 5 S L13

FILE 'REGISTRY' ENTERED AT 14:43:23 ON 14 JUN 2006
L15 1 S 114554-11-9/RN

L16 FILE 'CAPLUS' ENTERED AT 14:43:23 ON 14 JUN 2006
3 S L15

L17 FILE 'REGISTRY' ENTERED AT 14:43:24 ON 14 JUN 2006
1 S 115503-79-2/RN

L18 FILE 'CAPLUS' ENTERED AT 14:43:24 ON 14 JUN 2006
5 S L17

L19 FILE 'REGISTRY' ENTERED AT 14:43:25 ON 14 JUN 2006
1 S 119643-82-2/RN

L20 FILE 'CAPLUS' ENTERED AT 14:43:25 ON 14 JUN 2006
13 S L19

L21 FILE 'REGISTRY' ENTERED AT 14:43:26 ON 14 JUN 2006
1 S 126298-92-8/RN

L22 FILE 'CAPLUS' ENTERED AT 14:43:26 ON 14 JUN 2006
4 S L21

L23 FILE 'REGISTRY' ENTERED AT 14:43:27 ON 14 JUN 2006
1 S 218443-88-0/RN

L24 FILE 'CAPLUS' ENTERED AT 14:43:28 ON 14 JUN 2006
3 S L23

L25 FILE 'REGISTRY' ENTERED AT 14:43:28 ON 14 JUN 2006
1 S 218443-90-4/RN

L26 FILE 'CAPLUS' ENTERED AT 14:43:29 ON 14 JUN 2006
2 S L25

L27 FILE 'REGISTRY' ENTERED AT 14:43:29 ON 14 JUN 2006
1 S 218443-91-5/RN

L28 FILE 'CAPLUS' ENTERED AT 14:43:30 ON 14 JUN 2006
2 S L27

L29 FILE 'REGISTRY' ENTERED AT 14:43:30 ON 14 JUN 2006
1 S 218443-92-6/RN

L30 FILE 'CAPLUS' ENTERED AT 14:43:31 ON 14 JUN 2006
2 S L29

L31 FILE 'REGISTRY' ENTERED AT 14:43:31 ON 14 JUN 2006
1 S 218443-93-7/RN

L32 FILE 'CAPLUS' ENTERED AT 14:43:32 ON 14 JUN 2006
2 S L31

L33 33 S L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 O
S 17750-23-1/REG# OR 7145-37-1/REG# OR 6456-44-6/REG# OR 546

L34 FILE 'REGISTRY' ENTERED AT 14:45:25 ON 14 JUN 2006
1 S 218443-88-0/RN

L35 FILE 'CAPLUS' ENTERED AT 14:45:25 ON 14 JUN 2006
3 S L34

L36 FILE 'REGISTRY' ENTERED AT 14:45:26 ON 14 JUN 2006
1 S 218443-90-4/RN

FILE 'CAPLUS' ENTERED AT 14:45:26 ON 14 JUN 2006

L37 2 S L36
 FILE 'REGISTRY' ENTERED AT 14:45:27 ON 14 JUN 2006
 L38 1 S 218443-91-5/RN
 FILE 'CAPLUS' ENTERED AT 14:45:27 ON 14 JUN 2006
 L39 2 S L38
 FILE 'REGISTRY' ENTERED AT 14:45:28 ON 14 JUN 2006
 L40 1 S 218443-92-6/RN
 FILE 'CAPLUS' ENTERED AT 14:45:28 ON 14 JUN 2006
 L41 2 S L40
 FILE 'REGISTRY' ENTERED AT 14:45:29 ON 14 JUN 2006
 L42 1 S 667919-86-0/RN
 FILE 'CAPLUS' ENTERED AT 14:45:29 ON 14 JUN 2006
 L43 39 S L42
 FILE 'REGISTRY' ENTERED AT 14:45:30 ON 14 JUN 2006
 L44 1 S 952-92-1/RN
 FILE 'CAPLUS' ENTERED AT 14:45:30 ON 14 JUN 2006
 L45 584 S L44
 FILE 'REGISTRY' ENTERED AT 14:45:31 ON 14 JUN 2006
 L46 1 S 4229-56-5/RN
 FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
 L47 77 S L46
 FILE 'REGISTRY' ENTERED AT 14:45:32 ON 14 JUN 2006
 L48 1 S 5463-59-2/RN
 FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
 L49 18 S L48
 FILE 'REGISTRY' ENTERED AT 14:45:33 ON 14 JUN 2006
 L50 1 S 6456-44-6/RN
 FILE 'CAPLUS' ENTERED AT 14:45:33 ON 14 JUN 2006
 L51 104 S L50
 FILE 'REGISTRY' ENTERED AT 14:45:34 ON 14 JUN 2006
 L52 1 S 7145-37-1/RN
 FILE 'CAPLUS' ENTERED AT 14:45:34 ON 14 JUN 2006
 L53 6 S L52
 FILE 'REGISTRY' ENTERED AT 14:45:35 ON 14 JUN 2006
 L54 1 S 17750-23-1/RN
 FILE 'CAPLUS' ENTERED AT 14:45:35 ON 14 JUN 2006
 L55 107 S L54
 L56 878 S L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 O
 => s l33 or l56
 L57 898 L33 OR L56
 => s CB (2W) 1954
 12521 CB
 3998 CBS
 16198 CB

(CB OR CBS)
8267 1954
L58 95 CB (2W) 1954

=> s CB (2W) 1954/cn

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
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PROXIMITY OPERATOR LEVEL NOT CONSISTENT WITH
FIELD CODE - 'AND' OPERATOR ASSUMED 'CB (2W) 1954/CN'

L60 0 L59

=> s cb1954

L61 104 CB1954

=> s cb-1954

12521 CB

3998 CBS

16198 CB

(CB OR CBS)

8267 1954

L62 95 CB-1954

(CB(W) 1954)

=> s l62 or l61

L63 178 L62 OR L61

=> s l63 and l57

L64 18 L63 AND L57

=> s l64 not py>1997

8391976 PY>1997

L65 9 L64 NOT PY>1997

=> s l64 not py>1996

9151625 PY>1996

L66 7 L64 NOT PY>1996

=> d ibib 1-7

L66 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:203 CAPLUS

DOCUMENT NUMBER: 120:203

TITLE: Identification, synthesis and properties of
5-(aziridin-1-yl)-2-nitro-4-nitrosobenzamide, a novel
DNA crosslinking agent derived from **CB1954**

AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Biggs, Patrick J.;
Flitter, William D.; Gaskell, Margaret; Goddard,
Phyllis; Davies, Lawrence; Jarman, Michael

CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res.,
Sutton/Surrey, SM2 5NG, UK

SOURCE: Biochemical Pharmacology (1993), 46(5), 797-803

CODEN: BCPA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

L66 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:93913 CAPLUS
DOCUMENT NUMBER: 118:93913
TITLE: The bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB1954**). II. A comparison of an Escherichia coli nitroreductase and Walker DT diaphorase
AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Sherwood, Roger F.; Melton, Roger G.; Anlezark, Gillian M.
CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SOURCE: Biochemical Pharmacology (1992), 44(12), 2297-301
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:165847 CAPLUS
DOCUMENT NUMBER: 116:165847
TITLE: The differences in kinetics of rat and human DT diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide) [Erratum to document cited in CA115(1):332c].
AUTHOR(S): Boland, Marion P.; Knox, Richard J.; Roberts, John J.
CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SOURCE: Biochemical Pharmacology (1991), 42(Suppl.), S229
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:34040 CAPLUS
DOCUMENT NUMBER: 116:34040
TITLE: Bioactivation of **CB 1954**: reaction of the active 4-hydroxylamino derivative with thioesters to form the ultimate DNA-DNA interstrand crosslinking species
AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Marchbank, Tania; Roberts, John J.
CORPORATE SOURCE: Sect. Drug Dev., Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
SOURCE: Biochemical Pharmacology (1991), 42(9), 1691-7
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:421743 CAPLUS
DOCUMENT NUMBER: 115:21743
TITLE: Cytotoxicity and activation of **CB1954** in a human tumor cell line
AUTHOR(S): Sunters, Andrew; Baer, John; Bagshawe, Kenneth D.
CORPORATE SOURCE: Dep. Med. Oncol., Charing Cross Hosp., London, W6 8RF, UK
SOURCE: Biochemical Pharmacology (1991), 41(9), 1293-8
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

L66 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:400332 CAPLUS
DOCUMENT NUMBER: 115:332
TITLE: The differences in kinetics of rat and human DT

diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide)
 AUTHOR(S): Boland, Marion P.; Knox, Richard J.; Roberts, John J.
 CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK
 SOURCE: Biochemical Pharmacology (1991), 41(6-7), 867-75
 CODEN: BCPA6; ISSN: 0006-2952
 DOCUMENT TYPE: Journal
 LANGUAGE: English

L66 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1989:128164 CAPLUS

DOCUMENT NUMBER: 110:128164

TITLE: A new cytotoxic, DNA interstrand crosslinking agent, 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide, is formed from 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB 1954**) by a nitroreductase enzyme in Walker carcinoma cells

AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Jarman, Michael; Roberts, John J.

CORPORATE SOURCE: Mol. Pharmacol. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5NG, UK

SOURCE: Biochemical Pharmacology (1988), 37(24), 4661-9
 CODEN: BCPA6; ISSN: 0006-2952

DOCUMENT TYPE: Journal

LANGUAGE: English

=> d kwic 5

L66 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Cytotoxicity and activation of **CB1954** in a human tumor cell line

AB **CB1954** (5-aziridin-1-yl-2,4-dinitrobenzamide) is a monofunctional alkylating agent, to which Walker 256 cells are very sensitive. These cells express a nitroreductase which reduces **CB1954** to a bifunctional crosslinking agent 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. In vitro testing on the human colon line LS174T showed that the differential cytotoxicities between the monofunctional agent (**CB1954**), and the active species (generated in situ by the addition of NADH and the Walker rat nitroreductase) were smaller than anticipated due to the unexpected toxicity of **CB1954** (IC50 value for **CB1954** on LS174T cells of 78 µM). The toxicity of the chemical synthesized active form was less than if it had. . an enzyme of similar mol. weight to that of the 33 kD Walker cell nitroreductase, which is capable of reducing **CB1954** to its toxic metabolite, and reducing MTT to its insol. formazan salt. The expression of this enzyme presumably accounts for the unexpected toxicity of **CB1954**.

ST **CB 1954** cytotoxicity activation colon tumor

IT Intestine, neoplasm

(colon, **CB1954** cytotoxicity and activation in)

IT 9037-41-6, Nitroreductase

RL: BIOL (Biological study)

(**CB1954** activation by, in human colon tumor cells)

IT 21919-05-1, **CB1954**

RL: PROC (Process)

(cytotoxicity and activation of, in human colon tumor cells)

IT 119643-82-2

RL: PROC (Process)

(cytotoxicity and formation of, from **CB1954**, in human colon tumor cells)

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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DICTIONARY FILE UPDATES: 13 JUN 2006 HIGHEST RN 887650-39-7

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* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
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<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 119643-82-2/RN

L67 1 119643-82-2/RN

=> SET NOTICE 1 DISPLAY

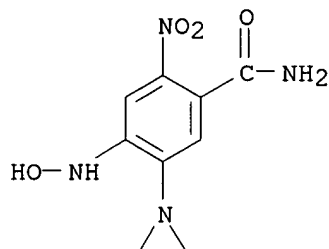
NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L67 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L67 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 119643-82-2 REGISTRY

CN Benzamide, 5-(1-aziridinyl)-4-(hydroxyamino)-2-nitro- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C9 H10 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPATFULL
 DT.CA CAplus document type: Journal; Patent
 RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)
 RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1907 TO DATE)
 13 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
 SET COMMAND COMPLETED

=>

=> file caplus

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FULL ESTIMATED COST	2.34	219.13
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.75

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=> d 166 kwic 1-7

L66 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Identification, synthesis and properties of 5-(aziridin-1-yl)-2-nitro-4-nitrosobenzamide, a novel DNA crosslinking agent derived from **CB1954**

AB 5-(Aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide, the active form of the antitumor agent 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB1954**), can react spontaneously with oxygen, and in aqueous solution yields 5-(aziridin-1-yl)-2-nitro-4-nitrosobenzamide and hydrogen peroxide. In order to understand fully the bioactivation of **CB1954**, chemical and biol. properties of the nitroso compound were studied. Mild biol. reducing agents such as NAD(P)H, reduced thiols, and. . . synthesis of 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide are described. These results emphasize the potential efficacy of the in situ activation of prodrugs such as **CB1954** either by endogenous enzymes such as DT diaphorase, or by antibody directed enzyme prodrug therapy (ADEPT).
ST antitumor aziridinyldinitrobenzamide bioactivation product cytotoxicity; DNA crosslinking antitumor **CB1954** bioactivation product; hydroxylaminobenzamide prepn cytotoxicity DNA crosslinking; nitrosobenzamide prepn cytotoxicity DNA crosslinking

IT Neoplasm inhibitors

(**CB1954** and its bioactivation products)

IT Deoxyribonucleic acids

RL: RCT (Reactant); RACT (Reactant or reagent)

(interstrand crosslinking of, by **CB1954** bioactivation products)

IT 21919-05-1, **CB1954**

RL: BIOL (Biological study)

(bioactivation products of, antitumor activity and cytotoxicity and DNA crosslinking by)

IT **119643-82-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antitumor activity of, as **CB1954** active form)

IT 151602-22-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and antitumor activity of, as **CB1954** product)

L66 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI The bioactivation of 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB1954**). II. A comparison of an Escherichia coli nitroreductase and Walker DT diaphorase

AB A nitroreductase enzyme that has been isolated from Escherichia coli B is capable of bioactivating **CB1954** [5-(aziridin-1-yl)-2,4-dinitrobenzamide] to a cytotoxic agent, a property shared with the mammalian enzyme Walker DT diaphorase [NAD(P)H dehydrogenase (quinone), EC 1.6.99.2] as isolated from Walker cells. In contrast to Walker DT diaphorase, which can only reduce the 4-nitro group of **CB1954**, the E. coli nitroreductase can reduce either (but not both) nitro groups of **CB1954** to the corresponding hydroxylamino species. The two hydroxylamino species are formed in equal proportions and at the same rates. **CB1954** is reduced much more rapidly by the E. coli

nitroreductase than by Walker DT diaphorase. If the reduction of **CB1954** was carried out in the presence of V79 cells (which are insensitive to **CB1954**) a large cytotoxic effect was evident. This cytotoxicity was only observed under conditions in which the E. coli nitroreductase or. . . proposed that E. coli B nitroreductase would be a suitable enzyme for antibody-directed enzyme prodrug therapy (ADEPT) in combination with **CB1954**.

IT 119643-82-2 119643-83-3

RL: FORM (Formation, nonpreparative)

(formation of, from aziridinyl dinitrobenzamide by nitroreductase of E. coli, antitumor activity in relation to)

L66 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI The differences in kinetics of rat and human DT diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide) [Erratum to document cited in CAl15(1):332c].

IT 119643-82-2

RL: FORM (Formation, nonpreparative)

(formation of, from **CB 1954**, DT diaphorase of humans and laboratory animals induction of (Erratum))

IT 9032-20-6

RL: PRP (Properties)

(kinetics of, of human and laboratory animal, differential sensitivity of tumors cells to **CB 1954** in relation to (Erratum))

L66 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Bioactivation of **CB 1954**: reaction of the active 4-hydroxylamino derivative with thioesters to form the ultimate DNA-DNA interstrand crosslinking species

AB 5-(Aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide (I) is the active form of **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide).

This hydroxylamine is formed by the bioedn. of **CB 1954**

by the enzyme DT diaphorase and accounts for the highly selective

cytotoxicity of this compound The reason why the hydroxylamine derivative is

so

cytotoxic is that, in contrast to **CB 1954**, it can react difunctionally as characterized by the formation of DNA-DNA interstrand crosslinks in cells treated by this agent. However,. . . DNA reactive species was a minor product of the reaction. It is proposed that the ultimate, DNA reactive, derivative of **CB 1954** is 4-(N-acetoxy)-5-(aziridin-1-yl)-2-nitrobenzamide.

ST **CB 1954** bioactivation DNA crosslinking cytotoxicity

IT Neoplasm inhibitors

(**CB 1954** as, bioactivation in, DNA interstrand crosslinking in)

IT Deoxyribonucleic acids

RL: RCT (Reactant); RACT (Reactant or reagent)

(interstrand crosslinking of, by **CB 1954**

bioactivation product, cytotoxicity in relation to)

IT Carboxylic acids, esters

RL: BIOL (Biological study)

(thio-, esters, **CB 1954** active metabolite binding to DNA response to, cytotoxicity in relation to)

IT 72-89-9, Acetyl coenzyme A 70019-69-1 70019-70-4

RL: BIOL (Biological study)

(**CB 1954** active metabolite binding to DNA response to, cytotoxicity in relation to)

IT 9032-20-6, DT Diaphorase

RL: BIOL (Biological study)

(**CB 1954** bioactivation by, DNA interstrand

crosslinking from, thioesters in, cytotoxicity in relation to)

IT 21919-05-1, **CB 1954**

RL: BIOL (Biological study)

(bioactivation of, DNA-DNA interstrand crosslinking in, thioesters in)
 IT 1866-15-5, S-Acetylthiocholine iodide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with **CB 1954** active metabolite, DNA crosslinking in, cytotoxicity in relation to)
 IT 119643-82-2
 RL: BIOL (Biological study)
 (reaction with DNA of, as **CB 1954** metabolite, thioesters effect on, cytotoxicity in relation to)

L66 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Cytotoxicity and activation of **CB1954** in a human tumor cell line
 AB **CB1954** (5-aziridin-1-yl-2,4-dinitrobenzamide) is a monofunctional alkylating agent, to which Walker 256 cells are very sensitive. These cells express a nitroreductase which reduces **CB1954** to a bifunctional crosslinking agent 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. In vitro testing on the human colon line LS174T showed that the differential cytotoxicities between the monofunctional agent (**CB1954**), and the active species (generated in situ by the addition of NADH and the Walker rat nitroreductase) were smaller than anticipated due to the unexpected toxicity of **CB1954** (IC50 value for **CB1954** on LS174T cells of 78 μ M). The toxicity of the chemical synthesized active form was less than if it had. . an enzyme of similar mol. weight to that of the 33 kD Walker cell nitroreductase, which is capable of reducing **CB1954** to its toxic metabolite, and reducing MTT to its insol. formazan salt. The expression of this enzyme presumably accounts for the unexpected toxicity of **CB1954**.

ST **CB 1954** cytotoxicity activation colon tumor
 IT Intestine, neoplasm
 (colon, **CB1954** cytotoxicity and activation in)
 IT 9037-41-6, Nitroreductase
 RL: BIOL (Biological study)
 (**CB1954** activation by, in human colon tumor cells)
 IT 21919-05-1, **CB1954**
 RL: PROC (Process)
 (cytotoxicity and activation of, in human colon tumor cells)
 IT 119643-82-2
 RL: PROC (Process)
 (cytotoxicity and formation of, from **CB1954**, in human colon tumor cells)

L66 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI The differences in kinetics of rat and human DT diaphorase result in a differential sensitivity of derived cell lines to **CB 1954** (5-(aziridin-1-yl)-2,4-dinitrobenzamide)
 AB DT diaphorase (NAD(P)H dehydrogenase (quinone), EC 1.6.99.2) isolated from Walker 256 rat carcinoma cells can convert **CB 1954** to a cytotoxic DNA interstrand crosslinking agent. This is achieved by reduction of the 4-nitro group of **CB 1954** to produce the hydroxylamino species, a bioactivation which accounts for the much greater sensitivity of Walker cells to **CB 1954** when compared with other cells which are unable to carry out this reduction. As predicted from their measured DT diaphorase activities a number of rat hepatoma and hepatocyte cell lines were also shown to be sensitive to **CB 1954**. However, no **CB 1954**-sensitive cell lines of human origin were found, although levels of DT diaphorase similar to those in the sensitive rat cells were present in these cells. The human cells were as sensitive as rat cells to the active form of **CB 1954** (5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide). DT diaphorase, purified to homogeneity from human Hep G2 cells, did metabolize **CB 1954** to this 4-hydroxylamino product, but the rate of **CB 1954** reduction and thus production of the cytotoxic product, was much lower than that of purified Walker

enzyme (ratio of Kcat = 6.4). In addition, **CB 1954** could be considered an inhibitor of, rather than a substrate for, the human form of DT diaphorase. The purified rat and human DT diaphorases possessed otherwise similar biochem. and mol. properties. These findings explain the decreased sensitivity towards **CB 1954** of human cell lines when compared to rat cell lines.

IT **119643-82-2**

RL: FORM (Formation, nonpreparative)
(formation of, from **CB 1954**, DT diaphorase of humans and laboratory animals induction of)

IT 9032-20-6

RL: PRP (Properties)
(kinetics of, of human and laboratory animal, differential sensitivity of tumors cells to **CB 1954** in relation to)

IT 21919-05-1, **CB 1954**

RL: BIOL (Biological study)
(tumor sensitivity to, of humans and laboratory animals, DT diaphorase kinetics in relation to)

L66 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI A new cytotoxic, DNA interstrand crosslinking agent, 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide, is formed from 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB 1954**) by a nitroreductase enzyme in Walker carcinoma cells

AB Walker tumor cells in vivo or in vitro are exceptionally sensitive to the monofunctional alkylating agent **CB 1954**. **CB 1954** forms DNA interstrand crosslinks in a time-dependent manner in Walker tumor cells but not in nontoxically affected Chinese hamster V79 cells. However, coculturing Chinese hamster V79 cells with Walker cells in the presence of **CB 1954** rendered the hamster cells sensitive to **CB 1954** and led to the formation of interstrand crosslinks in their DNA, findings indicative of the formation by Walker cells of a diffusible toxic metabolite of **CB 1954**. A flavoprotein, of mol. weight 33.5 kDa as estimated by SDS-polyacrylamide gel electrophoresis, was isolated from Walker cells and identified. . . dehydrogenase (quinone) (DT diaphorase, EC 1.6.99.2). This enzyme, in the presence of NADH or NADPH, catalyzed the aerobic reduction of **CB 1954** to 5-(aziridin-1-yl)-4-hydroxylamino-2-nitrobenzamide. This new compound can form interstrand crosslinks in the DNA of Chinese hamster V79 cells to which it. . .

ST **CB 1954** antitumor NADPH dehydrogenase prepn

IT Deoxyribonucleic acids

RL: RCT (Reactant); RACT (Reactant or reagent)
(crosslinking of, by **CB 1954**, metabolism by NADPH dehydrogenase in)

IT Neoplasm inhibitors

(carcinoma, **CB 1954** as, metabolism by NADPH dehydrogenase in)

IT 9032-20-6, NAD(P)H dehydrogenase

RL: BIOL (Biological study)
(**CB 1954** metabolism to antitumor metabolite by)

IT **119643-82-2**

RL: FORM (Formation, nonpreparative)
(formation of, as **CB 1954** antitumor metabolite)

IT 21919-05-1, **CB 1954**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(neoplasm inhibition by, DNA crosslinking by metabolite in)

IT 61837-23-8P 61837-26-1P 119643-83-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and formation as **CB 1954** metabolite of, neoplasm inhibition in relation to)

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	13.29	232.42
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.50	-5.25

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STRUCTURE FILE UPDATES: 13 JUN 2006 HIGHEST RN 887650-39-7
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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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conducting SmartSELECT searches.

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*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
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Structure search iteration limits have been increased. See HELP SLIMITS
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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> S 119643-83-3/RN

L68 1 119643-83-3/RN

=> SET NOTICE 1 DISPLAY

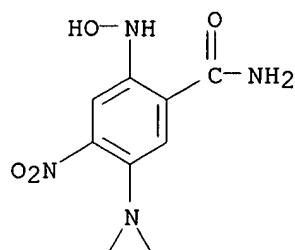
NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

=> D L68 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L68 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 119643-83-3 REGISTRY
 CN Benzamide, 5-(1-aziridinyl)-2-(hydroxyamino)-4-nitro- (9CI) (CA INDEX NAME)
 MF C9 H10 N4 O4
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
 6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
 SET COMMAND COMPLETED

=>

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.34	234.76
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.25

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 FILE LAST UPDATED: 13 Jun 2006 (20060613/ED)

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L1 FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006
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SEL RN

L2 FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006
45 S E1-E45

L3 FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006
64271 S L2
L4 145 S PRODRUG (L) L3

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L5 FILE 'REGISTRY' ENTERED AT 14:43:18 ON 14 JUN 2006
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4 S L5

L7 FILE 'REGISTRY' ENTERED AT 14:43:19 ON 14 JUN 2006
1 S 97009-81-9/RN

L8 FILE 'CAPLUS' ENTERED AT 14:43:19 ON 14 JUN 2006
12 S L7

L9 FILE 'REGISTRY' ENTERED AT 14:43:20 ON 14 JUN 2006
1 S 99362-74-0/RN

L10 FILE 'CAPLUS' ENTERED AT 14:43:20 ON 14 JUN 2006
3 S L9

L11 FILE 'REGISTRY' ENTERED AT 14:43:21 ON 14 JUN 2006
1 S 106047-77-2/RN

L12 FILE 'CAPLUS' ENTERED AT 14:43:21 ON 14 JUN 2006
4 S L11

L13 FILE 'REGISTRY' ENTERED AT 14:43:22 ON 14 JUN 2006
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3 S L15

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 L58 95 S CB (2W) 1954
 S CB (2W) 1954/CN
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 L59 0 S CB (2W) 1954/CN
 FILE 'CAPLUS' ENTERED AT 14:46:25 ON 14 JUN 2006

L60 0 S L59
L61 104 S CB1954
L62 95 S CB-1954
L63 178 S L62 OR L61
L64 18 S L63 AND L57
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L66 7 S L64 NOT PY>1996

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L67 1 S 119643-82-2/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

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L68 1 S 119643-83-3/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

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=> s 157 not 119643-82-2

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L70 13 L69

L71 885 L57 NOT L70

=> s 171 and prodrug
10858 PRODRUG
10801 PRODRUGS
15241 PRODRUG
(PRODRUG OR PRODRUGS)

L72 6 L71 AND PRODRUG

=> d ibib 1-6

L72 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:301733 CAPLUS

DOCUMENT NUMBER: 141:306746

TITLE: Quinone reductase-mediated nitro-reduction: clinical applications

AUTHOR(S): Knox, Richard J.; Chen, Shiuan

CORPORATE SOURCE: Enact Pharma PLC, Salisbury, SP4 0JQ, UK

SOURCE: Methods in Enzymology (2004), 382(Quinones and Quinone Enzymes, Part B), 194-221

CODEN: MENZAU; ISSN: 0076-6879

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

REFERENCE COUNT: 92 THERE ARE 92 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:749515 CAPLUS
DOCUMENT NUMBER: 140:121861
TITLE: CB 1954: From the Walker tumor to NQO2 and VDEPT
AUTHOR(S): Knox, Richard J.; Burke, Philip J.; Chen, Shiuan;
Kerr, David J.
CORPORATE SOURCE: Enact Pharma PLC, Salisbury, UK
SOURCE: Current Pharmaceutical Design (2003), 9(26), 2091-2104
CODEN: CPDEFP; ISSN: 1381-6128
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:835107 CAPLUS
DOCUMENT NUMBER: 139:414
TITLE: Improved cancer treatment with enzyme technology
CORPORATE SOURCE: Enact Pharma, Enact Pharma plc, Salisbury, SP4 0JQ, UK
SOURCE: sp2 (2002), 1(8), 22, 24-25
CODEN: SPSUCF; ISSN: 1476-184X
PUBLISHER: Avakado Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

L72 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:584913 CAPLUS
DOCUMENT NUMBER: 135:338611
TITLE: Aerobic nitroreduction by flavoproteins: enzyme
structure, mechanisms and role in cancer chemotherapy
AUTHOR(S): Skelly, Jane V.; Knox, Richard J.; Jenkins, Terence C.
CORPORATE SOURCE: School of Chemical and Life Sciences, University of
Greenwich, London, SE18 6PF, UK
SOURCE: Mini-Reviews in Medicinal Chemistry (2001), 1(3),
293-306
CODEN: MMCIAE; ISSN: 1389-5575
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:597759 CAPLUS
DOCUMENT NUMBER: 133:275962
TITLE: Bioactivation of 5-(aziridin-1-yl)-2,4-
dinitrobenzamide (CB 1954) by human NAD(P)H quinone
oxidoreductase 2: a novel co-substrate-mediated
antitumor **prodrug** therapy
AUTHOR(S): Knox, Richard J.; Jenkins, Terence C.; Hobbs, Stephen
M.; Chen, Shiuan; Melton, Roger G.; Burke, Philip J.
CORPORATE SOURCE: Enact Pharma Plc, Salisbury, SP4 0JQ, UK
SOURCE: Cancer Research (2000), 60(15), 4179-4186
CODEN: CNREA8; ISSN: 0008-5472
PUBLISHER: American Association for Cancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L72 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:124026 CAPLUS
DOCUMENT NUMBER: 130:306493

TITLE: Formation of N-methylnicotinamide in the brain from a dihydropyridine-type **prodrug**: effect on brain choline

AUTHOR(S): Erb, Christina; Seidel, Albrecht; Frank, Heinz; Platt, Karl L.; Oesch, Franz; Klein, Jochen

CORPORATE SOURCE: Department of Pharmacology, University of Mainz, Mainz, D'55101, Germany

SOURCE: Biochemical Pharmacology (1999), 57(6), 681-684
CODEN: BCPA6; ISSN: 0006-2952

PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s 21919-05-1

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L74 176 L73

=> d his

(FILE 'HOME' ENTERED AT 14:30:32 ON 14 JUN 2006)

FILE 'CAPLUS' ENTERED AT 14:30:42 ON 14 JUN 2006

L1 1 S US 20030086933/PN
SEL RN

FILE 'REGISTRY' ENTERED AT 14:30:57 ON 14 JUN 2006

L2 45 S E1-E45

FILE 'CAPLUS' ENTERED AT 14:32:35 ON 14 JUN 2006

L3 64271 S L2
L4 145 S PRODRUG (L) L3

FILE 'CAPLUS' ENTERED AT 14:40:17 ON 14 JUN 2006

S 218443-93-7/REG# OR 218443-92-6/REG# OR 218443-91-5/REG# OR

FILE 'REGISTRY' ENTERED AT 14:43:18 ON 14 JUN 2006

L5 1 S 89080-16-0/RN

FILE 'CAPLUS' ENTERED AT 14:43:18 ON 14 JUN 2006

L6 4 S L5

FILE 'REGISTRY' ENTERED AT 14:43:19 ON 14 JUN 2006

L7 1 S 97009-81-9/RN

FILE 'CAPLUS' ENTERED AT 14:43:19 ON 14 JUN 2006

L8 12 S L7

FILE 'REGISTRY' ENTERED AT 14:43:20 ON 14 JUN 2006

L9 1 S 99362-74-0/RN

FILE 'CAPLUS' ENTERED AT 14:43:20 ON 14 JUN 2006

L10 3 S L9

L11 FILE 'REGISTRY' ENTERED AT 14:43:21 ON 14 JUN 2006
 1 S 106047-77-2/RN

L12 FILE 'CAPLUS' ENTERED AT 14:43:21 ON 14 JUN 2006
 4 S L11

L13 FILE 'REGISTRY' ENTERED AT 14:43:22 ON 14 JUN 2006
 1 S 109942-74-7/RN

L14 FILE 'CAPLUS' ENTERED AT 14:43:22 ON 14 JUN 2006
 5 S L13

L15 FILE 'REGISTRY' ENTERED AT 14:43:23 ON 14 JUN 2006
 1 S 114554-11-9/RN

L16 FILE 'CAPLUS' ENTERED AT 14:43:23 ON 14 JUN 2006
 3 S L15

L17 FILE 'REGISTRY' ENTERED AT 14:43:24 ON 14 JUN 2006
 1 S 115503-79-2/RN

L18 FILE 'CAPLUS' ENTERED AT 14:43:24 ON 14 JUN 2006
 5 S L17

L19 FILE 'REGISTRY' ENTERED AT 14:43:25 ON 14 JUN 2006
 1 S 119643-82-2/RN

L20 FILE 'CAPLUS' ENTERED AT 14:43:25 ON 14 JUN 2006
 13 S L19

L21 FILE 'REGISTRY' ENTERED AT 14:43:26 ON 14 JUN 2006
 1 S 126298-92-8/RN

L22 FILE 'CAPLUS' ENTERED AT 14:43:26 ON 14 JUN 2006
 4 S L21

L23 FILE 'REGISTRY' ENTERED AT 14:43:27 ON 14 JUN 2006
 1 S 218443-88-0/RN

L24 FILE 'CAPLUS' ENTERED AT 14:43:28 ON 14 JUN 2006
 3 S L23

L25 FILE 'REGISTRY' ENTERED AT 14:43:28 ON 14 JUN 2006
 1 S 218443-90-4/RN

L26 FILE 'CAPLUS' ENTERED AT 14:43:29 ON 14 JUN 2006
 2 S L25

L27 FILE 'REGISTRY' ENTERED AT 14:43:29 ON 14 JUN 2006
 1 S 218443-91-5/RN

L28 FILE 'CAPLUS' ENTERED AT 14:43:30 ON 14 JUN 2006
 2 S L27

L29 FILE 'REGISTRY' ENTERED AT 14:43:30 ON 14 JUN 2006
 1 S 218443-92-6/RN

L30 FILE 'CAPLUS' ENTERED AT 14:43:31 ON 14 JUN 2006
 2 S L29

L31 FILE 'REGISTRY' ENTERED AT 14:43:31 ON 14 JUN 2006
 1 S 218443-93-7/RN

L32 FILE 'CAPLUS' ENTERED AT 14:43:32 ON 14 JUN 2006
2 S L31
L33 33 S L32 OR L30 OR L28 OR L26 OR L24 OR L22 OR L20 OR L18 OR L16 O
S 17750-23-1/REG# OR 7145-37-1/REG# OR 6456-44-6/REG# OR 546

L34 FILE 'REGISTRY' ENTERED AT 14:45:25 ON 14 JUN 2006
1 S 218443-88-0/RN

L35 FILE 'CAPLUS' ENTERED AT 14:45:25 ON 14 JUN 2006
3 S L34

L36 FILE 'REGISTRY' ENTERED AT 14:45:26 ON 14 JUN 2006
1 S 218443-90-4/RN

L37 FILE 'CAPLUS' ENTERED AT 14:45:26 ON 14 JUN 2006
2 S L36

L38 FILE 'REGISTRY' ENTERED AT 14:45:27 ON 14 JUN 2006
1 S 218443-91-5/RN

L39 FILE 'CAPLUS' ENTERED AT 14:45:27 ON 14 JUN 2006
2 S L38

L40 FILE 'REGISTRY' ENTERED AT 14:45:28 ON 14 JUN 2006
1 S 218443-92-6/RN

L41 FILE 'CAPLUS' ENTERED AT 14:45:28 ON 14 JUN 2006
2 S L40

L42 FILE 'REGISTRY' ENTERED AT 14:45:29 ON 14 JUN 2006
1 S 667919-86-0/RN

L43 FILE 'CAPLUS' ENTERED AT 14:45:29 ON 14 JUN 2006
39 S L42

L44 FILE 'REGISTRY' ENTERED AT 14:45:30 ON 14 JUN 2006
1 S 952-92-1/RN

L45 FILE 'CAPLUS' ENTERED AT 14:45:30 ON 14 JUN 2006
584 S L44

L46 FILE 'REGISTRY' ENTERED AT 14:45:31 ON 14 JUN 2006
1 S 4229-56-5/RN

L47 FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
77 S L46

L48 FILE 'REGISTRY' ENTERED AT 14:45:32 ON 14 JUN 2006
1 S 5463-59-2/RN

L49 FILE 'CAPLUS' ENTERED AT 14:45:32 ON 14 JUN 2006
18 S L48

L50 FILE 'REGISTRY' ENTERED AT 14:45:33 ON 14 JUN 2006
1 S 6456-44-6/RN

L51 FILE 'CAPLUS' ENTERED AT 14:45:33 ON 14 JUN 2006
104 S L50

L52 FILE 'REGISTRY' ENTERED AT 14:45:34 ON 14 JUN 2006
1 S 7145-37-1/RN

FILE 'CAPLUS' ENTERED AT 14:45:34 ON 14 JUN 2006


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L53          6 S L52

FILE 'REGISTRY' ENTERED AT 14:45:35 ON 14 JUN 2006
L54          1 S 17750-23-1/RN

FILE 'CAPLUS' ENTERED AT 14:45:35 ON 14 JUN 2006
L55          107 S L54
L56          878 S L55 OR L53 OR L51 OR L49 OR L47 OR L45 OR L43 OR L41 OR L39 O
L57          898 S L33 OR L56
L58          95 S CB (2W) 1954
              S CB (2W) 1954/CN

FILE 'REGISTRY' ENTERED AT 14:46:25 ON 14 JUN 2006
L59          0 S CB (2W) 1954/CN

FILE 'CAPLUS' ENTERED AT 14:46:25 ON 14 JUN 2006
L60          0 S L59
L61          104 S CB1954
L62          95 S CB-1954
L63          178 S L62 OR L61
L64          18 S L63 AND L57
L65          9 S L64 NOT PY>1997
L66          7 S L64 NOT PY>1996

FILE 'REGISTRY' ENTERED AT 14:49:42 ON 14 JUN 2006
L67          1 S 119643-82-2/RN
              SET NOTICE 1 DISPLAY
              SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 14:50:09 ON 14 JUN 2006

FILE 'REGISTRY' ENTERED AT 14:51:48 ON 14 JUN 2006
L68          1 S 119643-83-3/RN
              SET NOTICE 1 DISPLAY
              SET NOTICE LOGIN DISPLAY

FILE 'CAPLUS' ENTERED AT 14:52:04 ON 14 JUN 2006
              S L57 NOT 119643-82-2/REG#

FILE 'REGISTRY' ENTERED AT 14:52:47 ON 14 JUN 2006
L69          1 S 119643-82-2/RN

FILE 'CAPLUS' ENTERED AT 14:52:48 ON 14 JUN 2006
L70          13 S L69
L71          885 S L57 NOT L70
L72          6 S L71 AND PRODRUG
              S 21919-05-1/REG#

FILE 'REGISTRY' ENTERED AT 14:54:26 ON 14 JUN 2006
L73          1 S 21919-05-1/RN

FILE 'CAPLUS' ENTERED AT 14:54:26 ON 14 JUN 2006
L74          176 S L73

=> s 174 or 163
L75          201 L74 OR L63

=> s 175 not 163
L76          23 L75 NOT L63

=> s 176 and 171
L77          0 L76 AND L71

=> s methylnicotinamide

```

1670 METHYLNICOTINAMIDE
11 METHYLNICOTINAMIDES
L78 1676 METHYLNICOTINAMIDE
(METHYLNICOTINAMIDE OR METHYLNICOTINAMIDES)

=> s 178 and 175
L79 2 L78 AND L75

=> d ibib 1-2

L79 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:620223 CAPLUS
DOCUMENT NUMBER: 123:25632
TITLE: Virtual cofactors for an Escherichia coli
nitroreductase enzyme: relevance to reductively
activated prodrugs in antibody directed enzyme prodrug
therapy (ADEPT)
AUTHOR(S): Knox, Richard J.; Friedlos, Frank; Jarman, Michael;
Davies, Lawrence C.; Goddard, Phyllis; Anlezark,
Gillian M.; Melton, Roger G.; Sherwood, Roger F.
CORPORATE SOURCE: Cent. Cancer Therapeutics, Inst. Cancer Res.,
Sutton/Surrey, UK
SOURCE: Biochemical Pharmacology (1995), 49(11), 1641-7
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

L79 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:566472 CAPLUS
DOCUMENT NUMBER: 117:166472
TITLE: Identification of novel reduced pyridinium derivatives
as synthetic cofactors for the enzyme DT diaphorase
(NAD(P)H dehydrogenase (quinone), EC 1.6.99.2)
AUTHOR(S): Friedlos, Frank; Jarman, Michael; Davies, Lawrence C.;
Boland, Marion P.; Knox, Richard J.
CORPORATE SOURCE: Sect. Drug Dev., Inst. Cancer Res., Sutton/Surrey, SM2
5NG, UK
SOURCE: Biochemical Pharmacology (1992), 44(1), 25-31
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

=> d abs kwic 1-2

L79 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
AB A nitroreductase enzyme has been isolated from Escherichia coli that has
the unusual property of being equally capable of using either NADH or
NADPH as a cofactor for the reduction of its substrates which include
menadione as well as 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB**
1954). This property is shared with the mammalian enzyme, DT
diaphorase. The nitroreductase can, like DT diaphorase, also use simple
reduced pyridinium compds. as virtual cofactors. The intact NAD(P)H mol.
is not required and the simplest quaternary (and therefore reducible)
derivative of nicotinamide, 1-methylnicotinamide (reduced), is as
effective as NAD(P)H in its ability to act as an electron donor for the
nitroreductase. The structure-activity relation is not identical to that
of DT diaphorase and nicotinic acid riboside (reduced) is selective, being
active only for the nitroreductase. Irresp. of the virtual cofactor used,
the nitroreductase formed the same reduction products of **CB**
1954 (the 2- and 4-hydroxylamino derivs. in equal proportions).
Nicotinic acid riboside (reduced), unlike NADH, was stable to metabolism by
serum enzymes and had a plasma half-life of seven minutes in the mouse

after an i.v. bolus administration. NADH had an unmeasurably short half-life. Nicotinic acid riboside (reduced) could also be produced in vivo by administration of nicotinic acid 5'-O-benzoyl riboside (reduced). These results demonstrate that the requirement for a cofactor need not be a limitation in the use of reductive enzymes in antibody directed enzyme prodrug therapy (ADEPT). It is proposed that the E. coli nitroreductase would be a suitable enzyme for ADEPT in combination with **CB 1954** and a synthetic, enzyme-selective, virtual cofactor such as nicotinic acid riboside (reduced).

AB . . . either NADH or NADPH as a cofactor for the reduction of its substrates which include menadione as well as 5-(aziridin-1-yl)-2,4-dinitrobenzamide (**CB 1954**). This property is shared with the mammalian enzyme, DT diaphorase. The nitroreductase can, like DT diaphorase, also use simple reduced. . . as virtual cofactors. The intact NAD(P)H mol. is not required and the simplest quaternary (and therefore reducible) derivative of nicotinamide, 1-methylnicotinamide (reduced), is as effective as NAD(P)H in its ability to act as an electron donor for the nitroreductase. The structure-activity. . . being active only for the nitroreductase. Irresp. of the virtual cofactor used, the nitroreductase formed the same reduction products of **CB 1954** (the 2- and 4-hydroxylamino derivs. in equal proportions). Nicotinic acid riboside (reduced), unlike NADH, was stable to metabolism by serum. . . therapy (ADEPT). It is proposed that the E. coli nitroreductase would be a suitable enzyme for ADEPT in combination with **CB 1954** and a synthetic, enzyme-selective, virtual cofactor such as nicotinic acid riboside (reduced).

L79 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

AB The enzyme DT diaphorase [NAD(P)H dehydrogenase (quinone), EC 1.6.99.2] is unusual in that it can utilize either NADH or NADPH as a cofactor for the reduction of its substrates. It was previously shown that the intact NAD(P)H mol. is not required and that other reduced pyridinium compds. can also act as cofactors for DT diaphorase. The entire adenine dinucleotide portion of NAD(P)H can be dispensed with entirely and the simplest quaternary (and therefore reducible) derivative of nicotinamide, 1-methylnicotinamide, was as effective as NAD(P)H as a co-factor for the reduction of the quinone, menadione. Nicotinamide 5'-O-benzoyl riboside was also as effective a cofactor as NAD(P)H, while nicotinamide ribotide and riboside have a higher Km, and decreased kcat with DT diaphorase. Nicotinic acid derivs. had little activity. Kinetic anal. indicated that both nicotinamide ribotide and riboside may be interacting with the menadione binding site rather than the NAD(P)H site. Irresp. of the differences between the various reduced pyridinium derivs. in their ability to act as cofactors for the reduction of menadione by DT diaphorase, all the compds. that showed activity in this assay were equally effective co-factors for the reduction of the nitrobenzamide, **CB 1954** [5-(aziridin-1-yl)-2,4-dinitrobenzamide]. The apparent Km of DT diaphorase for all these cofactors approached zero. It was concluded that cofactor binding is not a rate-limiting step in the nitroreductase activity of DT diaphorase.

AB . . . adenine dinucleotide portion of NAD(P)H can be dispensed with entirely and the simplest quaternary (and therefore reducible) derivative of nicotinamide, 1-methylnicotinamide, was as effective as NAD(P)H as a co-factor for the reduction of the quinone, menadione. Nicotinamide 5'-O-benzoyl riboside was also. . . diaphorase, all the compds. that showed activity in this assay were equally effective co-factors for the reduction of the nitrobenzamide, **CB 1954** [5-(aziridin-1-yl)-2,4-dinitrobenzamide]. The apparent Km of DT diaphorase for all these cofactors approached zero. It was concluded that cofactor binding is. . .

IT 21919-05-1

RL: BIOL (Biological study)

(reaction of DT diaphorase of Walker 256 tumor cells, reduced pyridinium derivs. as cofactors for)

IT 53-57-6, NADPH 58-68-4, NADH 86-08-8, 3-Acetylpyridineadenine
 dinucleotide 321-02-8, Nicotinic acid ribotide 1094-61-7, Nicotinamide
 ribotide 1341-23-7, Nicotinamide riboside 3106-60-3, 1-
Methylnicotinamide 5869-54-5, α -NADH 6704-97-8
 17720-18-2 32095-01-5 80658-03-3, α -NADPH 143613-19-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with DT diaphorase of Walker 256 tumor cells, kinetics
 of)

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	13.85	262.07
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.50	-6.75

STN INTERNATIONAL LOGOFF AT 14:59:37 ON 14 JUN 2006